Supplementary materials

A)





B)





Figure S1: Chromatographic UHPLC profiles of crude extract of *S.latissima* extracted by (**A**) water, (**B**) aqueous ethanol (30% v/v), and (**C**) aqueous ethanol (80% v/v). The UHPLC profile was run at three different wavelengths.



Figure S2: Chromatographic UHPLC profiles of phloroglucinol as standard at the concentrations of 50, 100, 200, and 500 mg/L. The UHPLC profile was run at three different wavelengths.



A)



B)



Figure S3: Chromatographic UHPLC profiles of lyophilized purified extracts (1 g/L) from *S*. *latissima*, extracted by (**A**) water, (**B**) aqueous ethanol (30% v/v), and (**C**) aqueous ethanol (80% v/v). The UHPLC profile was run at three different wavelengths.

•



A)



Figure S4: Chromatographic UHPLC profiles of lyophilized purified extracts (1 g/L) of *A. nodosum* extracted by (A) aqueous ethanol (30% v/v), and (B) aqueous ethanol (80% v/v). The UHPLC profile was run at three different wavelengths.



Figure S5: Chromatographic UHPLC profiles of sugars in extracts of *S. latissima* extracted by (**A**) water, (**B**) aqueous ethanol (30% v/v), and (**C**) aqueous ethanol (80% v/v).



Figure S6: A. Extracted ion-chromatogram of *m*/*z* 389.0509 found in *A. nodosum*, **B.** Comparison of detected (top) and calculated (bottom) isotopes for *m*/*z* 389.0509 found in *A. nodosum*.



Figure S7: A. Extracted ion-chromatogram of *m*/*z* 497.0719 found in *A. nodosum*, **B.** Comparison of detected (top) and calculated (bottom) isotopes for *m*/*z* 497.0719 found in *A. nodosum*.



Figure S8: A. Extracted ion-chromatogram of *m*/*z* 621.0869 found in *A. nodosum*, **B.** Comparison of detected (top) and calculated (bottom) isotopes for *m*/*z* 621.0875 found in *A. nodosum*.



Figure S9: A. Extracted ion-chromatogram of *m*/*z* 745.1026 found in *A. nodosum*, **B.** Comparison of detected (top) and calculated (bottom) isotopes for *m*/*z* 745.1027 found in *A. nodosum*.



Figure S10: MS¹ and MS² spectra of *m*/*z* 497.0720 found in *A. nodosum*.



Figure S11: MS¹ and MS² spectra of m/z 621.0875 found in *A. nodosum*.

Table S1: MZmine 2 settings to create peak lists

- 1. Peak detection
 - 1.2 Mass detection function
 - 1.2.1 Settings:
 - 1.2.1.1 Polarity: negative
 - 1.2.1.2 Mass detector: exact mass
 - 1.2.1.3 Spectrum type: any
- 2. FTMS shoulder peaks filter
 - 2.2 Settings:
 - 2.2.1 Mass resolution: 100000
 - 2.2.2 Peak model function: Lorentzian extended
- 3. Chromatogram builder
 - 3.2 Settings:
 - 3.2.1 Min time span (min): 0.10
 - 3.2.2 Min height: 5.0E3
 - 3.2.3 *m*/*z* tolerance: 0.01 *m*/*z*
- 4. Chromatogram deconvolution
 - 4.2 Settings:
 - 4.2.1 Algorithm: local minimum search
 - 4.2.1.1 Chromatographic threshold: 80%
 - 4.2.1.2 Search minimum in retention time range (min): 0.20
 - 4.2.1.3 Minimum relative height: 1%
 - 4.2.1.4 Minimum absolute height: 5.0E3
 - 4.2.1.5 Min ratio of peak top/edge: 2
 - 4.2.1.6 Peak duration range (time): 0.00 10.00
 - 4.2.2 m/z center calculation: Median
- 5. Isotopic peak grouper
 - 5.2 Settings:
 - 5.2.1 *m*/*z* tolerance: 0.005 *m*/*z*
 - 5.2.2 Retention time tolerance: 0.2 min
 - 5.2.3 Maximum charge: 2
 - 5.2.4 Representative isotope: most intense
- 6. Chemical formula prediction
 - 6.2 Settings:
 - 6.2.1 Charge: 1
 - 6.2.2 Ionization type: [M-H]-
 - 6.2.3 *m*/*z* tolerance: 0.05 *m*/*z*
 - 6.2.4 Max best formulas per peak: 3
 - 6.2.5 Elements
 - 6.2.5.1 C (min: 0; max 100)

- 6.2.5.2 O (min: 0; max 100)
- 6.2.5.3 H (min: 0; max 100)

6.2.6 Element count heuristics

- 6.2.6.1 H/C ratio: on
- 6.2.6.2 NOPS/C ratios: off
- 6.2.6.3 Multiple element counts: on
- 6.2.7 RDBE restrictions
 - 6.2.7.1 RDBE range: -1 to 40
 - 6.2.7.2 RDBE must be an integer: yes
- 6.2.8 Isotopic pattern filter:
 - 6.2.8.1 Isotope *m*/*z* tolerance: 0.005 *m*/*z*
 - 6.2.8.2 Minimum absolute intensity: 1.0E3

Minimum score: 80.0%